Diethylene glycol diethyl ether 112-36-7 | DTXSID3025047

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 98.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 8.02e-01

Nearest Neighbors from the Training Set

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Ethyl heptanoate Measured: 407 Predicted: 284 Image not found

Aldicarb

Measured: 31.6 Predicted: 38.0 Image not found

Ethyl hexanoate Measured: 115 Predicted: 110

Image not found

2-Phenylethyl acetate Measured: 77.6 Predicted: 98.8 Image not found

Ethyl phenylacetate Measured: 77.6 Predicted: 103